To: Judson, Richard[Judson.Richard@epa.gov]; Martin, Matt[Martin.Matt@epa.gov]
From: Wambaugh, John
Sent: Tue 7/30/2013 1:31:05 PM
Subject: Rat AUCs
RDynamic_0.8.tar.gz
vLiverPBPK_0.8.tar.gz
PredictedAUC-073013.RData

Hi Richard -- I am able to piece together AUC predictions for 115 Phase I chemicals. Right now all the AUCs are for 28 day studies at 1 mg/kg BW/day. The predictions are stored by CAS number is vLiver.rat.values.

If you need a different dose than 1 mg/kg BW/day, just multiply the value -- this model is linear in dose.

If you need a different study duration you will need to rerun the model (pretty fast, if I do say so myself). Here is the code I used to loop over all the chemicals with sufficient data to make a PBPK model (get_PBPK_CAS()):

```
library(vLiverPBPK)

study.duration <- rep(28,length(get_PBPK_CAS()))
names(study.duration) <- get_PBPK_CAS()

vLiver.rat.values <- NULL
for (this.CAS in get_PBPK_CAS())
{
  these.params <- parameterize_vLiverPBPK(this.CAS,species="Rat")
  if (these.params[["Fraction_unbound_plasma"]] < 0.01)
these.params[["Fraction_unbound_plasma"]] <- 0.005
  vLiver.rat.values[[this.CAS]] <-
calc_dailydose_AUC(these.params,days=study.duration[[this.CAS]],dose=1)
}
```

Just change the study duration for a given CAS and rerun the loop.

Please let me know if you run into any snags -- this is code that has generally not been

used by other people so it may have a lot of weirdness.

John

John Wambaugh
National Center for Computational Toxicology
US EPA, Mail Code B205-01
Research Triangle Park, NC 27711
Wambaugh.John@epa.gov
919-541-7641